PADSTE HIGHLIGHTS June 14, 2006

BIOSCIENCES

Recent *Proceedings of the National Academy of Sciences* paper highlighted on *Science Daily* website

Recent work by Paul Langan, Leighton Coates, Benno Schoenborn (all in BIO-CBSBFC) and collaborators not only appeared in the ***Proceedings of the National Academy of Sciences***, but was also featured in the popular online magazine ***Science Daily***. The research highlighted an innovative collaboration between Bioscience Division, the Fox Chase Cancer Center and the University of Tennessee that used the Protein Crystallography Station (PCS) at LANSCE to demonstrate that neutron diffraction can be used to model the enzyme D-xylose isomerase and to locate the elusive hydrogen atoms in its binding region, or active site.

Determining the structure and function of enzymes (specialized proteins involved in basic cell processes) is difficult because of the critical importance of hydrogen atoms in the active site, which are practically invisible to traditional visualization methods such as x-ray crystallography. Fortunately, the PCS at LANL offers the world's only spallation neutron source for protein diffraction studies, a method that makes it possible to identify the role hydrogen atoms play in the enzyme's functionality. D-xylose isomerase is a valuable commercial enzyme for the conversion of glucose to fructose – needed to create corn syrup – and knowing more detail about how the enzyme works could help increase reaction rates. Furthermore, understanding the mechanism of this enzyme's function may also be valuable for cancer research.

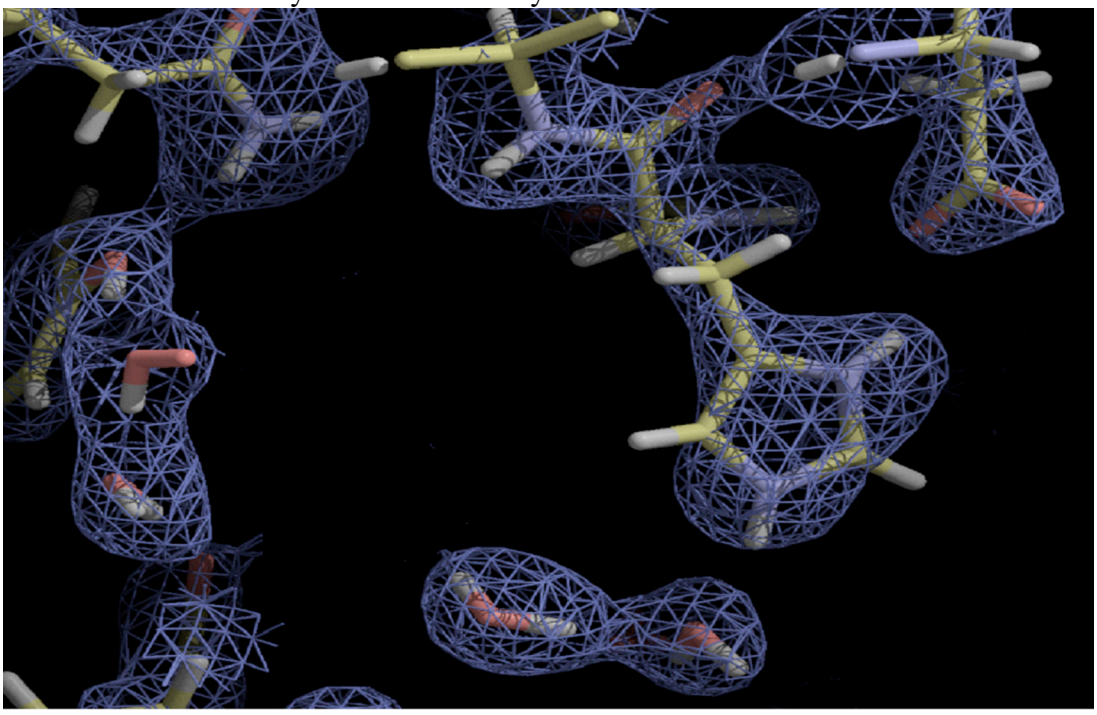


Figure 1. The graphics show nuclear density in the active site of D-xylose isomerase calculated from neutron diffraction data collected on the Protein Crystallography Station at LANSCE.

Diagnostic Test Evaluation Study for Department of Homeland Security (DHS)
Last week, the Homeland Security and Defense (HSD) Program office (previously called CHS) assembled a team from T, BIO, N, DA, EES, ISR, and ENVP Divisions for a quick turn around study for DHS to determine the sampling and processing demands for the National Laboratory Response Network (LRN) during an outbreak of pandemic flu in human and animal populations or an anthrax attack on multiple cities. This study was funded by a DHS/S&T project that pre-positioned funds at LANL to provide rapid analysis on hot topics of national security. DHS supplied specific outbreak scenarios to the team and asked for an estimate over time of the number of diagnostic LRN tests that would be needed across the country. The effort involved a careful analysis of the current national sampling strategies from over 1000 hospitals nationally and from special response teams during and after an event. The conclusion was that events of this magnitude challenge the current surge capacity of the LRN. The detailed findings of this effort were delivered to DHS/S&T Tuesday after two days of analysis. The ability to assemble rapidly a diverse team on almost any topic to provide input at a national planning level illustrates the utility of the large, multi-discipline national labs in supporting national security for biodefense. Team members included: Norman L. Johnson (HSD), Lead; Benjamin H. McMahon (T-TBB), Norman A. Doggett (BIO-GSCB), Helen Cui (N-SSS), Jeanne M. Fair (EES-ACED), Jennifer M. Rudnick (BIO-DO), Paul W. Fenimore (T-TBB), David R Janecky (ENVP-AQE), Michael J. Brown (DA-SEI), Steve P. Linger (DA-EIA), Jennifer Watkins (T-TBB).

CHEMISTRY

Chemistry Work Captures *Science News* Cover
The work of C-PCS's Rich Schaller and Victor Klimov was featured on the cover of the June 3rd edition of the weekly magazine ***Science News***. Schaller and Klimov are exploring ways of using nanocrystal quantum dots to multiply the output of solar cells. Ordinary solar cells exposed to sunlight produce a single electron per photon, but semiconductor nanocrystals respond to photons with multiple electrons. The potential implications for the solar power industry are tremendous and have been generating much excitement in the news. The complete ***Science News*** article can be found online in the June 3, 2006 edition. Volume 169, No. 22.
http://www.sciencenews.org/articles/20060603/bob8.asp

Schaller and Klimov are members of the Softmatter Nanotechnology and Advanced Spectroscopy Team. Klimov is the team leader, and Schaller is a staff member on the team. More information about the researchers and their work is available on the Softmatter Nanotechnology and Advanced Spectroscopy Team web site http://quantumdot.lanl.gov/ and on the Chemistry Division Research Highlights web page at

http://pearl1.lanl.gov/external/research.htm

Sunrise over the Sangre de Cristo Mountains. Photo by Josh Smith, C-DO.

EARTH AND ENVIRONMENTAL SCIENCE

***Vadose Zone Journal* Names Brent Newman as 2005 Outstanding Associate Editor**
Brent Newman (EES-ACED) was selected as the 2005 Outstanding Associate Editor by the ***Vadose Zone Journal*** for his editorial contributions to a special issue of ***Vadose Zone Journal*** in August, 2005. The citation as printed in Crop Science of America News and on the American Society of Agronomy's web site reads, "In addition, the ***Vadose Zone Journal*** recognized Brent Newman of Los Alamos National Laboratory as its 2005 Outstanding Associate Editor.

Newman's work on the LANL special section featured in the August 2005 issue in particular exemplified his leadership and dedication to quality."

Collaboration with Landcare Institute, New Zealand

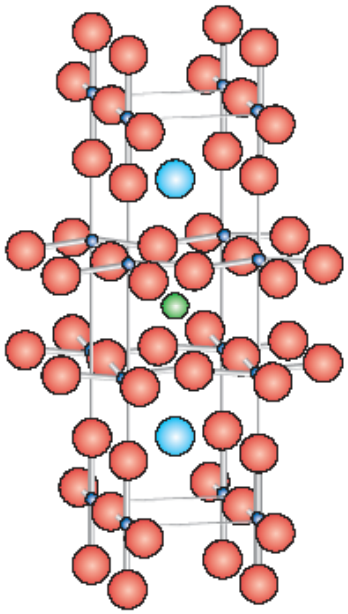
Nate McDowell (EES-ACED) traveled to New Zealand this spring to continue collaborations with Margaret Barbour of Landcare Institute. This trip was a reciprocal trip that was funded by the government of New Zealand and builds on a trip Barbour made to Los Alamos in 2005. McDowell and Barbour have two papers in review, and more research in progress from their collaboration on oxygen-18 flux in ecosystems including the Piñon-Juniper woodlands at TA-51. The oxygen-18 measurements will provide novel insight into carbon-water coupling in drought stressed ecosystems, a fundamental gap in our knowledge of the mechanisms of tree mortality and drought response.

Workshop on National Seismic Hazards Maps

Jamie Gardner of Environmental Geology and Spatial Analysis (EES-EGSA) was an invited participant at the Workshop for Updating the National Seismic Hazards Maps, Intermountain West Region in Reno, Nevada, May 31 and June 1. The workshop was organized by the U. S. Geological Survey and co-hosted by the University of Nevada, Reno. The meeting covered new information on seismic sources, attenuation relations, geodetic data, seismicity, and engineering and seismic zonation issues. Results of the workshop will contribute to changes in the updated National Seismic Hazards Maps, which provide a basis for national seismic zonation and building codes.

MATERIALS PHYSICS AND APPLICATIONS

MPA-STC research cause for optimism for application of High Temperature Superconductivity (HTS) materials



MPA-STC research on magnetic flux pinning was called out in a recent ***Nature Materials*** editorial as a reason for optimism for application of high-temperature superconducting materials. "Hot Superconductors, 20 years on" (***Nature Mater.*** **5,** 419; 2006) references "Strongly enhanced current densities in superconducting coated conductors of $YBa_2Cu_3O_{7-x}$ + $BaZrO_3$," (***Nature Mater.*** **3,** 439–443; 2004) by Judith Macmanus-Driscoll *et al*. The article is based on her research when she was on sabbatical in the MST Superconducting Technology Center (STC) and has been cited more than 50 times. Co-authors include Stephen Foltyn, Quanxi Jia, Haiyan Wang, Leonardo Civale, Boris Maiorov, Martin Maley, Dean Peterson, (all MPA-STC); Adriana Serquis (formerly of MST-STC), and Marilyn Hawley (MST-SPR). The researchers embedded nanoparticles of $BaZrO_3$ in the lattice to enhance magnetic flux pinning and thus improve in-magnetic field current density in conductors that are already of high quality. The DOE – Office of Energy Efficiency and Renewable Energy, supported the research.

Figure 3. The structure of the classic high-temperature superconductor, $YBa_2Cu_3O_7$ (known as YBCO). Yttrium is green, barium light blue, copper dark blue, and oxygen red.

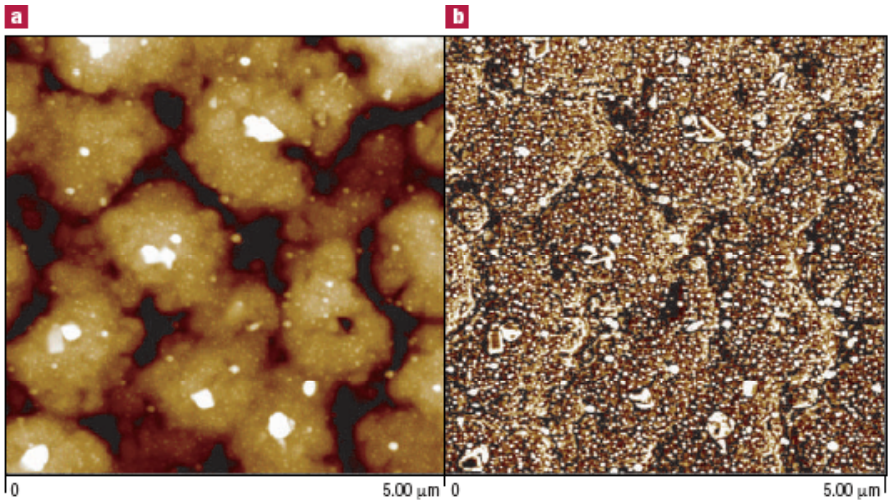


Figure 4. Micrographs of YBCO + $BaZrO_3$ films grown on single crystal $SrTiO_3$ showing surface nanoparticles. a, Atomic force micrograph and b, phase contrast micrograph.

MATERIALS SCIENCE AND TECHNOLOGY

Visiting professor to investigate crystallographic pitting

Prof. Emad El Din Abd El Aal is visiting MST-MTM's Corrosion - Electrochemistry Team for a sabbatical through December. Prof. Abd El Aal is currently a professor of physical chemistry, in the Department of Chemistry at Zagazig University, Zagazig, Egypt. He has an extensive publication record in the fields of electrode reactions, electrode kinetics and oxide film growth, corrosion and corrosion inhibition of metals, as well as initiation and inhibition of pitting corrosion in copper, nickel, lead, and zinc. During his sabbatical he will work with Scott Lillard (MST-MTM) in the area of localized corrosion. Specifically, Prof Abd El Aal hopes to contribute to the understanding of crystallographic pitting, a form of corrosion frequently observed in beryllium. He will use experimental techniques, such as electrochemical scanning tunneling microscopy, to study crystallographic pitting. Prof Abd El Aal became aware of MST's capacity in this field through international societies and journal publications.

MST-MTM team meets critical milestone for hydro shot

MST-MTM's Foundry, Machining and Mechanical Fabrication Team recently delivered a gold object for hydro shot 3624.This object will help certify the diagnostics at the Dual Axis Radiographic Hydrodynamic Test Facility (DARHT). The gold was cast in the MST-MTM foundry, and the part then machined in the Sigma machine shop. The final machining pass had 2.8 million lines of code and required a continuous run of 19 hours to complete. MST-MTM's John Balog and Rodina Lucero, an apprentice with the Los Alamos National Laboratory Machining Apprentice Program, were particularly instrumental in getting the object completed to meet this critical milestone. Also participating in the work were MST-MTM's Deniece Korzekwa (foundry/machining team leader), Robert Aikin, Tim Beard, Fermin Garcia, Manuel Jaramillo, Richard Less, Hunter Swenson, Ralph Trujillo; and apprentice Joseph Reichert.